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MONOENERGETIC NEUTRAL PARTICLE TRANSPORT IN SEMI-INFINITE MEDIA

CALSPAN - UB Research Center

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MONOENERGETIC NEUTRAL PARTICLE TRANSPORT IN SEMI-INFINITE MEDIA

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Abstract- A large class of half-space transport problems for neutral particles is considered including single and adjacent half-space geometries. Localized and distributed sources emitting particles either in a particular direction, isotropically or with a given angular distribution are considered. All solutions are based on the solution to the well-known albedo problem. A numerical Laplace transform inversion is used to generate highly accurate benchmark solutions which can be used to assess the error incurred by numerical transport algorithms.

I. INTRODUCTION

Particle transport theory had its inception with the establishment of the Boltzmann equation by Ludwig Boltzmann in the late nineteenth century[1]. In its most general form, the equation, which serves as the basis for many fields of physics, has evaded analytical solution. Only for special cases, i.e., the linear or linearized forms and simplified non-linear collision models, have

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analytical solutions been obtained. With today's computational power, however, the numerical solution to the Boltzmann equation for physically interesting cases in the linear and non-linear formulations can be obtained relatively easily. Various methods such as discrete ordinates, Legendre and other polynomial expansions, the F_N method, direct simulation Monte Carlo and other approximate methods have proven to provide adequate numerical solutions for certain applications. These methods, however, contain numerical approximations in various forms. The effect of these numerical errors usually goes unassessed and their influence on the desired result remains uncertain.

In 1953, the first comprehensive tool[2] attempting to provide standards to allow the assessment of numerical errors associated with approximate solutions to the linear neutral particle transport equation was published. This compilation is a collection of analytical solutions complete with numerical evaluations (some of which are unfortunately inaccurate) which could be used as standards or benchmarks to which approximate solutions could be compared. Infinite medium problems were emphasized in this collection because standard numerical methods at that time were considered reliable enough to adequately evaluate the analytical representations obtained for this class of problems.

It is now the nineties, almost 50 years since the first analytical benchmark compilation appeared. During that time there has been enormous progress made in the areas required for the generation of transport benchmarks, namely, in analytical and numerical methods development and computational power. This report is concerned with the development of the components required specifically for the generation of transport benchmarks in one-dimensional semi-infinite (half-space) plane geometry.

A fundamental problem in neutral particle transport theory concerns the collision of neutral particles with stationary scattering centers and

the subsequent streaming between collisions in a semi-infinite medium. The semi-infinite homogeneous medium is infinite in extent bordering either on a vacuum or another half-space of a different material. In general, upon collision with a scattering center (usually a molecule or nucleus), a particle will lose energy elastically or inelastically. For our purposes, we will consider only monoenergetic neutral particle transport which ignores inelastic scattering and assumes heavy scattering centers that can absorb an unlimited amount of momentum. For this case, neutral particles scatter and move between collisions with a constant velocity. Energy transfer considerations are usually handled through the multigroup formulation of which monoenergetic transport is a special case. In addition to the assumption of monoenergetic transport, we will assume that the neutral particle leaves a collision with no preferred direction which is the assumption of isotropic scattering.

Half-space transport problems first appeared in connection with photon transport in planetary atmospheres in the form of the Milne problem[3–5]. For this case, a source embedded deep within the interior of a star continuously emits an unlimited supply of photons, a portion of which exit the star's atmosphere. The curvature of the atmospheric surface can be neglected in comparison to the photon mean free path which allows a plane geometry approximation to be used. Variations based on the Milne problem soon appeared in the literature as part of neutron transport theory[6] where the source was moved to the free surface (called the albedo problem). Because of its simplicity and the fact that this problem contains the essential nature of neutral particle transport theory, the half-space problem has achieved prominance in the field. For this reason, monoenergetic neutral particle transport in a semi-infinite medium will be studied here and a collection of benchmarks will be presented.

One of the major themes of this investigation is the establishment of half-space solutions based solely on the solution to the single half-space albedo problem for an entering beam. It is remarkable that almost all solutions to half-space transport problems, including those for two dissimilar half-spaces, can be obtained from this one basic solution. Another pervasive theme found here is the ease with which truly accurate benchmarks can be generated. The key to the accuracy of the numerical evaluation is the numerical Laplace transform inversion which has recently been developed to solve the types of transport problems to be considered.

Single half-space problems including the albedo, Milne, and spatially-distributed sources will be considered in § II. The preferred method of solution is the Laplace transform and its inversion. The motivation for this choice is the desire to obtain useable numerical results rather than simply analytical representations. The solution representation for the angular and scalar (angularly integrated) fluxes can, in general, be expressed as contour integrals which can further be manipulated by analytic continuation if the singularities in the complex plane are known. Finding these singularities usually requires a significant computational effort which is avoided in the inversion procedure that has been developed. The numerical inversion is also applied to adjacent half-space problems which are considered in § III. Finally, in § IV the numerical implementation and demonstration of the solution technique is presented.

II. SINGLE HALF-SPACE SOLUTIONS

A single half-space bordering a vacuum will now be considered. The medium is assumed to be homogeneous and to contain scattering centers that scatter neutral particles isotropically. Physically, the assumption of isotropic scattering means that the direction of the "outgoing" particle after collision is randomly oriented and has no correlation with the direction of the "incoming" particle initiating the collision. In addition, as discussed in the introduction, the scattering interation does not change the particle energy (or velocity). Various source configurations will be considered including surface and spatially distributed sources and an embedded source infinitely far from the surface.

The single half-space problem is one of the fundamental problems of transport theory. It not only is of pedagogical interest but also has practical significance. In the non-destructive analysis of materials with high mass numbers, the reflected beam resulting from an impinging neutral beam can be used to infer material properties. The monoenergetic single half-space problem provides a first approximation to the reflected beam and can help guide the solution to the inverse problem from which the desired scattering characteristics of a medium can be inferred.

II.1 The Albedo Problem

For this problem, the source configuration is assumed to be particles impinging on the free surface of a homogeneous semi-infinite medium. If any absorption exists in the medium, then infinitely far from the surface the flux will vanish. However, if no absorption exists, then the flux will remain finite. Thus, for the following albedo problems considered for a variety of source angular distributions, the condition at infinity will be

$$\lim_{x \to \infty} \psi(x, \mu) \; < \; \infty \; , \; 0 \; \leq \; c \; \leq \; 1$$

where $\psi(x, \mu)$ is the directed or angular flux, c is the number of secondary (scattered) particles resulting from a collision and is explicitly given by

$$c \; = \; (\Sigma_s \; + \; \nu\Sigma_f)/\Sigma_t \; .$$

Σ_r represents the cross section (fractional probability per pathlength of travel) for process r where

$r = s$ scattering

$r = a$ absorption

$r = f$ fission

$r = t$ total ($\Sigma_t = \Sigma_a + \Sigma_s$) .

Fission is included for the case of neutrons with ν representing the number of neutrons produced in a fission.

The transport equation to be solved for the classic albedo problem is

$$\left[\mu \frac{\partial}{\partial x} \; + \; 1\right] \psi(x, \mu) \; = \; \frac{c}{2} \int_{-1}^{1} d\mu' \psi(x, \mu') \qquad (1a)$$

$$\psi(0, \mu) \; = \; f(\mu) \; , \; \mu \; > \; 0 \qquad (1b)$$

$$\lim_{x \to \infty} \psi(x, \mu) \; < \; \infty \qquad (1c)$$

where x is the position measured in units of mean free paths ($x = z\Sigma_t$, $z =$ actual position), μ is the particle direction cosine (referred to as the direction) and $f(\mu)$ is a general source distribution to be specified in the following subsections.

1.a. Entering Beam Flux

The solution to the albedo problem for a beam source serves as the basis for the solution to problems with the source configurations to follow. For this reason, the solution to the beam albedo problem will be presented in detail.

For a beam source,

$$f(\mu) = \delta(\mu - \mu_0) \ , \tag{2}$$

where the source is specified to be in direction μ_0 (which is actually a "cone" of incoming particles in the azimuthally symmetric plane geometry assumed).

i. Exiting flux

The exiting or reflected flux is likely to be the most important quantity to be determined. It also serves as the nucleus for the determination of the interior scalar flux as well as the angular flux. A sketch of the determination of an analytical expression for the exiting flux will now be given.

The procedure begins with the reformulation of eqs.(1) by following the particle along its trajectory to give for $\mu > 0$

$$\psi(x, \mu; \mu_0) = \delta(\mu - \mu_0)e^{-x/\mu_0} + \frac{c}{2\mu}\int_0^x dx' e^{-(x-x')/\mu}\psi(x'; \mu_0) \tag{3a}$$

and

$$\psi(x,-\mu;\mu_0) = \frac{c}{2\mu}\int_x^{\infty} dx' e^{-(x'-x)/\mu}\psi(x';\mu_0) \qquad (3b)$$

where the scalar flux is defined as

$$\psi(x;\mu_0) = \int_{-1}^{1} d\mu'\psi(x,\mu';\mu_0) \qquad (4)$$

and the dependence on μ_0 has been included for clarity. Then integrating eqs.(3a) and (3b) over μ on $[0,1]$ gives the following integral equation:

$$\psi(x;\mu_0) = e^{-x/\mu_0} + \frac{c}{2}\int_0^{\infty} dx' E_1(|\ x - x'\ |)\psi(x';\mu_0) \qquad (5)$$

where E_1 is the exponential integral defined by

$$E_1(x) = \int_0^1 \frac{d\mu}{\mu} e^{-x/\mu} \ .$$

This integral equation can be put in the more compact notation

$$(1 - L_x)\psi(x';\mu_0) = e^{-x/\mu_0} \qquad (6a)$$

where the operator L_x is

$$L_x \equiv \int_0^{\infty} dx' E_1(|\ x - x'\ |)(\cdot) \ . \qquad (6b)$$

Differentiating eq.(6a) with respect to x yields

$$(1 - L_x)\left[\frac{\partial}{\partial x'} + \frac{1}{\mu_0}\right]\psi(x';\mu_0) = \frac{c}{2}E_1(x)\psi(0;\mu_0) \qquad (7)$$

and also manipulating eq.(6a) gives

$$E_1(x) \;=\; (1 - L_x)\int_0^1 \frac{d\mu'}{\mu'}\psi(x';\mu')\;. \tag{8}$$

From eqs.(7) and (8), it is seen that the following expression is in the null space of the operator $1 - L_x$:

$$\left[\frac{\partial}{\partial x} \;+\; \frac{1}{\mu_0}\right]\psi(x;\mu_0) \;=\; \frac{c}{2}\psi(0;\mu_0)\int_0^1 \frac{d\mu'}{\mu'}\psi(x;\mu')\;. \tag{9}$$

The reciprocity relation,

$$\mu\psi(0,-\mu;\mu_0) \;=\; \mu_0\psi(0,-\mu_0;\mu)\;, \tag{10}$$

obtained from the self-adjointness of L_x, can be introduced into the result of multiplying eq.(9) by $e^{-x/\mu}$ and integrating over x to give [after liberal use of eq.(3b) with $x = 0$]

$$\psi(0,-\mu;\mu_0) \;=\; \frac{c}{2}\frac{\mu_0}{\mu + \mu_0}\psi(0;\mu_0)\psi(0;\mu)\;. \tag{11}$$

When this expression is introduced into the following representation of the scalar flux at $x = 0$ [eq.(4) with $x = 0$]

$$\psi(0;\mu_0) \;=\; 1 \;+\; \int_0^1 d\mu\psi(0,-\mu;\mu_0) \tag{12}$$

and defining the $H-$function by

$$H(\mu) \;=\; \psi(0;\mu)\;, \tag{13}$$

there results for the exiting flux

$$\psi(0,-\mu;\mu_0) \;=\; \frac{c}{2}\frac{\mu_0}{\mu+\mu_0}H(\mu_0)H(\mu)\;. \tag{14}$$

The Chandresekhar $H-$function[4] can be shown to satisfy the following non-linear integral equation

$$H(\mu) \;=\; 1 \;+\; \frac{c}{2}\mu H(\mu)\int_0^1 \; d\mu' \frac{H(\mu')}{\mu+\mu'} \tag{15}$$

which will serve as the basis for the numerical evaluation to be presented in § IV.

ii. Scalar flux

An expression is most easily obtained for the interior scalar flux $\psi(x)$ using eq.(3b) with $x = 0$

$$\psi(0,-\mu;\mu_0) \;=\; \frac{c}{2\mu}\int_0^\infty \; dx' \; e^{-x'/\mu}\psi(x';\mu_0)\;. \tag{16}$$

Noting that if μ is extended to the complex variable $1/s$, eq.(16) becomes a Laplace transform with the inversion

$$\psi(x;\mu_0) \;=\; \frac{2}{c}\mathcal{L}_x^{-1}\left[\psi(0,-1/s;\mu_0)/s\right] \tag{17}$$

where $\mathcal{L}_x^{-1}$ is the inverse Laplace transform operator

$$\mathcal{L}_x^{-1} \;\equiv\; \frac{1}{2\pi i}\int_{\gamma-i\infty}^{\gamma+i\infty} ds \; e^{sx}(\cdot)\;.$$

Since an analytical expression for the exiting flux already exists [eq.(14)], eq.(17) becomes

$$\psi(x;\mu_0) \;=\; \mu_0 H(\mu_0)\mathcal{L}_x^{-1}\left[\frac{H(1/s)}{1+\mu_0 s}\right] \qquad (18a)$$

with

$$H(1/s) \;=\; \left[1 \;-\; \frac{c}{2}\int_0^1 \; d\mu' \frac{H(\mu')}{1+\mu' s}\right]^{-1} \qquad (18b)$$

as obtained from eq.(15). Eq.(18a) can further be expanded by analytical continuation into the complex s-plane leading to contributions from pole and branch point singularities if desired. This will not be done here since the numerical inversion given in § IV will be applied directly to eq.(18a).

iii. Angular flux

The most straightforward way to obtain the angular flux is to apply the Laplace transform in x to the original transport equation [eqs.(1)] to give

$$(1+\mu s)\bar{\psi}(s,\mu;\mu_0) \;=\; \frac{c}{2}\bar{\psi}(s;\mu_0) + \mu\psi(0,\mu;\mu_0)\;. \qquad (19)$$

From eq.(17), by application of the Laplace transform, we have

$$\bar{\psi}(s;\mu_0) \;=\; \frac{2}{c}\psi(0,-1/s;\mu_0)/s\;, \qquad (20)$$

resulting in the transformed angular flux from eq.(19):

$$\bar{\psi}(s,\mu;\mu_0) \;=\; \frac{1}{1+\mu s}\left[\psi(0,-1/s;\mu_0)/s \;+\; \mu\psi(0,\mu;\mu_0)\right]\;. \qquad (21)$$

Thus, for $\mu > 0$

$$\bar{\psi}(s,\mu;\mu_0) \;=\; \frac{\mu_0}{1+\mu_0 s}\delta(\mu-\mu_0) \;+\; \frac{c}{2}\left[\frac{\mu_0 H(\mu_0)H(1/s)}{(1+\mu s)(1+\mu_0 s)}\right] \tag{22a}$$

and

$$\bar{\psi}(s,-\mu;\mu_0) \;=\; \frac{c}{2}\mu_0 H(\mu_0)\left[\frac{1}{1-\mu s}\left\{\frac{H(1/s)}{1+\mu_0 s} \;-\; \frac{H(\mu)}{1+\mu_0/\mu}\right\}\right] . \tag{22b}$$

The angular flux is therefore given by the inversion

$$\psi(x,\mu;\mu_0) \;=\; \mathcal{L}_x^{-1}\left[\bar{\psi}(s,\mu;\mu_0)\right] . \tag{23}$$

Again further manipulation is possible using analytical continuation into the complex s-plane but is not required in order to obtain reliable numerical results as will be shown.

1.b Entering Isotropic Flux

For an isotropic source, the boundary condition is

$$\psi(0,\mu) \;=\; 1 \;,\;\; \mu \;>\; 0 \,. \tag{24}$$

where the entering flux has been normalized to 1.

i. Exiting flux

The exiting flux for this case is obtained by integrating the result for the albedo problem over μ_0 on $[0,1]$

$$\psi(x,\mu) \;=\; \int_0^1 d\mu_0 \psi(x,\mu;\mu_0)\;, \tag{25}$$

to give

$$\psi(0,-\mu) \;=\; 1-\sqrt{1-c}\;H(\mu) \tag{26}$$

where the relation given by eq.(A.2) in Appendix A has been used.

ii. Scalar flux

At $x=0$, the scalar flux is

$$\psi(0) \;=\; \int_0^1 d\mu_0 H(\mu_0) \;=\; \frac{2}{c}(1-\sqrt{1-c}\;) \tag{27a}$$

using eq.(A.1). For $x>0$, the scalar flux is obtained by integrating eq.(18a) over μ_0 and using eq.(A.2) with μ replaced by $1/s$ to give

$$\psi(x) \;=\; \frac{2}{c}\mathcal{L}_x^{-1}\left[\left(1-\sqrt{1-c}\;H(1/s)\right)/s\right]\;. \tag{27b}$$

iii. Angular flux

Integrating eq.(21) over μ_0 gives

$$\bar{\psi}(s,\mu) \;=\; \frac{1}{1+\mu s}\left[\psi(0,-1/s)/s \;+\; \mu\psi(0,\mu)\right]\;; \tag{28}$$

and, therefore, for $\mu>0$ using eq.(26) as is and also with μ replaced by $1/s$, we have the transforms

$$\bar{\psi}(s,\mu) = \frac{\mu}{1+\mu s} + \frac{1}{s(1+\mu s)}\left[1 - \sqrt{1-c}\,H(1/s)\right] \tag{29a}$$

$$\psi(s,-\mu) = \frac{1}{1-\mu s}\left\{(1/s-\mu) - \sqrt{1-c}\left[H(1/s)/s - \mu H(\mu)\right]\right\} \tag{29b}$$

which are to be inverted.

1.c Entering Angularly Distributed Flux

For a general angularly distributed entering flux, the boundary condition is

$$\psi(0,\mu) = f(\mu)\ ,\ \text{for } \mu > 0\ .$$

This case, as for the previous case, is handled by noting that for an entering beam the flux is actually the "angular" (partial) Green's function; thus,

$$\psi(x,\mu) = \int_0^1 d\mu' f(\mu')\psi(x,\mu;\mu')\ . \tag{30}$$

i. Exiting flux

Using eq.(14), the exiting flux simply becomes

$$\psi(0,-\mu) = \frac{c}{2}H(\mu)\int_0^1 d\mu' \frac{\mu'}{\mu+\mu'} f(\mu')H(\mu')\ . \tag{31}$$

ii. Scalar flux

For $x = 0$,

$$\psi(0) = \int_0^1 d\mu' f(\mu')H(\mu') ; \tag{32a}$$

and for $x > 0$ from eqs.(30) and (18a)

$$\psi(x) = \mathcal{L}_x^{-1}\left[H(1/s)\int_0^1 d\mu' \frac{\mu'}{1+\mu' s} f(\mu')H(\mu')\right] . \tag{32b}$$

iii. Angular flux

Integrating eqs.(22) over μ_0 on $[0,1]$ weighted by f yields for $\mu > 0$

$$\bar{\psi}(s,\mu) = \frac{\mu}{1+\mu s} f(\mu) + \frac{c}{2}\frac{H(1/s)}{(1+\mu s)}\int_0^1 d\mu' \frac{\mu'}{1+\mu' s} f(\mu')H(\mu') \tag{33a}$$

$$\bar{\psi}(s,-\mu) = \frac{c}{2}\frac{1}{1-\mu s}\int_0^1 d\mu' \mu' f(\mu')H(\mu')\left[\frac{H(1/s)}{1+\mu' s} - \frac{H(\mu)}{1+\mu'/\mu}\right] \tag{33b}$$

with the inversion providing the angular flux as

$$\psi(x,\mu) = \mathcal{L}_x^{-1}\left[\bar{\psi}(s,\mu)\right] . \tag{34}$$

II.2 The Milne Problem

The Milne problem is one of the first half-space problems ever attempted. This problem found application in the determination of the photon current exiting the atmosphere of a star where the source is deeply embedded within the star's interior. For this case, the source is at infinity and must be of infinite strength itself in order to support a current infinitely far away exiting

the surface. The traditional condition taken at infinity is that the flux varies as the discrete eigenmode of the transport operator

$$\phi(x,\mu) \;\rightarrow \phi_{\nu_0}(-\mu)\; e^{x/\nu_0} \;, \text{ as x} \rightarrow \infty \tag{35a}$$

where

$$\phi_{\nu_0}(-\mu) \;=\; \frac{c}{2}\frac{\nu_0}{\mu+\nu_0} \;, \tag{35b}$$

and ν_0 is the solution to the dispersion relation

$$1 - \frac{c}{2}\nu_0 \;\ln\left(\frac{\nu_0+1}{\nu_0-1}\right) \;=\; 0 \;. \tag{35c}$$

The transport equation to be solved is therefore

$$\left[\mu\frac{\partial}{\partial x} \;+\; 1\right]\phi(x,\mu) \;=\; \frac{c}{2}\int_{-1}^{1} d\mu'\phi(x,\mu') \tag{36a}$$

$$\phi(0,\mu) \;=\; 0 \;,\; \mu > 0 \tag{36b}$$

$$\phi(x,\mu) \rightarrow \;\phi_{\nu_0}(-\mu)e^{x/\nu_0} \;, \text{ as x } \rightarrow \;\infty \tag{36c}$$

which is recast into a more convenient form by the substitution

$$\phi(x,\mu) \;=\; \phi_{\nu_0}(-\mu)\; e^{x/\nu_0} \;-\; \psi(x,\mu) \tag{37}$$

yielding

$$\left[\mu\frac{\partial}{\partial x} + 1\right]\psi(x,\mu) = \frac{c}{2}\int_{-1}^{1} d\mu'\psi(x,\mu') \tag{38a}$$

$$\psi(0,\mu) = \phi_{\nu_0}(-\mu)\ ,\ \mu > 0 \tag{38b}$$

$$\lim_{x\to\infty}\psi(x,\mu) = 0\ . \tag{38c}$$

It is this half-space problem which is to be solved based on the solution for the general angularly distributed entering flux found in § II.1.c.

2.a. Exiting flux

Since eqs.(38) represent a half-space problem with

$$f(\mu) = \phi_{\nu_0}(-\mu)\ ,$$

eq.(31) can be used directly to give

$$\psi(0,-\mu) = \left(\frac{c}{2}\right)^2 \nu_0 H(\mu)\int_0^1 d\mu'\frac{\mu'}{(\mu+\mu')(\nu_0+\mu')}H(\mu')\ . \tag{39}$$

Employing the identity

$$\frac{\mu'}{(\mu+\mu')(\nu_0+\mu')} = \frac{1}{\mu-\nu_0}\left[\frac{\mu}{\mu'+\mu} - \frac{\nu_0}{\mu'+\nu_0}\right]$$

and the integral equation for the $H-$ function [eq.(15)] gives the following (after some algebra):

$$\psi(0,-\mu) = \phi_{\nu_0}(\mu) - \frac{c}{2}\frac{\nu_0}{\nu_0-\mu}\frac{H(\mu)}{H(\nu_0)} \tag{40}$$

which when substituted into eq.(37) (with $x = 0$) yields the desired exiting flux

$$\phi(0,-\mu) \;=\; \frac{c}{2}\frac{\nu_0}{\nu_0-\mu}\frac{H(\mu)}{H(\nu_0)} \; . \tag{41}$$

2.b. Scalar flux

From integral transport theory, as found in § II.1,

$$\psi(0,-\mu) \;=\; \frac{c}{2\mu}\int_0^\infty dx' \; e^{-x'/\mu}\psi(x') \tag{42}$$

from which results (as previously noted)

$$\psi(x) \;=\; \frac{2}{c}\mathcal{L}_x^{-1}\left[\psi(0,-1/s)/s\right] \; .$$

Thus, form eq.(40)

$$\psi(x) \;=\; e^{x/\nu_0} \;-\; \frac{\nu_0}{H(\nu_0)}\mathcal{L}_x^{-1}\left[\frac{H(1/s)}{s\nu_0-1}\right] \tag{43}$$

and from eq.(37), integrated over μ noting that

$$\int_{-1}^{1} d\mu'\phi_{\nu_0}(-\mu') \;=\; 1 \; ,$$

there results

$$\phi(x) \;=\; \frac{\nu_0}{H(\nu_0)}\mathcal{L}_x^{-1}\left[\frac{H(1/s)}{s\nu_0-1}\right] \tag{44}$$

2.c. Angular flux

As before, the spatial transform of $\psi(x,\mu)$ is given by eq.(28) with ψ replaced by ϕ leading to for $\mu > 0$

$$\bar{\phi}(s,\mu) \;=\; \frac{c}{2}\frac{\nu_0}{(1+\mu s)(s\nu_0 - 1)}\frac{H(1/s)}{H(\nu_0)} \tag{45a}$$

$$\bar{\phi}(s,-\mu) \;=\; \frac{c}{2}\frac{\nu_0}{H(\nu_0)(1-\mu s)}\left[\frac{H(1/s)}{s\nu_0 - 1} - \frac{\mu H(\mu)}{\nu_0 - \mu}\right] \tag{45b}$$

with the angular flux again given by

$$\phi(x,\mu) \;=\; \mathcal{L}_x^{-1}\left[\bar{\phi}(s,\mu)\right] \; . \tag{46}$$

II.3 Spatially Distributed Sources

The half-space problem with a spatially distributed isotropically emitting source will be considered in this section. The appropriate transport equation to be solved is:

$$\left[\mu\frac{\partial}{\partial x} + 1\right]\phi(x,\mu) \;=\; \frac{c}{2}\int_{-1}^{1} d\mu'\phi(x,\mu') \;+\; \frac{Q(x)}{2} \tag{47a}$$

$$\phi(0,\mu) \;=\; 0 \; , \; \mu \; > \; 0 \tag{47b}$$

$$\lim_{x\to\infty}\phi(x,\mu) \;<\; \infty \; . \tag{47c}$$

The solution will again be obtained using the results of § II.1.a.

Starting with eqs.(1) for an entering beam flux and separating the uncollided from the collided contribution, we have

$$\psi(x,\mu;\mu_0) \;=\; \psi_0(x,\mu;\mu_0) \;+\; \psi_c(x,\mu;\mu_0) \; ; \tag{48}$$

and, therefore,

$$\left[\mu\frac{\partial}{\partial x} + 1\right]\psi_c(x,\mu;\mu_0) = \frac{c}{2}\int_{-1}^{1} d\mu'\psi_c(x,\mu';\mu_0) + \frac{c}{2}e^{-x/\mu_0} \quad (49a)$$

$$\psi_c(x,\mu;\mu_0) = 0\ ,\ \mu > 0 \quad (49b)$$

$$\lim_{x\to\infty}\psi_c(x,\mu;\mu_0) < \infty\ . \quad (49c)$$

If μ_0 is extended to the complex p-plane by replacing μ_0 by -$1/p$ and eqs.(49) are operated on by

$$\frac{1}{2\pi i}\int_{\gamma-i\infty}^{\gamma+i\infty} dp\ \bar{Q}(p)(\cdot)\ , \quad (50)$$

eqs.(49) become eqs.(47) with (from the uniqueness of the solution)

$$\phi(x,\mu) = \frac{1}{2\pi i}\frac{1}{c}\int_{\gamma-i\infty}^{\gamma+i\infty} dp\ \bar{Q}(p)\ \psi_c(x,\mu;-1/p) \quad (51)$$

where the Laplace transform of the source, $\bar{Q}(p)$, is assumed to only have singularities in the left half-plane for simplicity. It is this relation to the beam albedo problem that will be exploited in order to derive the results to follow.

3.a. Exiting flux

From eq.(51) with $x = 0$ and μ replaced by $-\mu$ and from eq.(14) with μ_0 replaced by $-1/p$ (note that the uncollided contribution is zero at $x = 0$),

$$\psi_c(0,-\mu;-1/p) = \frac{c}{2}\frac{H(\mu)H(-1/p)}{1-\mu p}\ , \quad (52)$$

there results

$$\phi(0,-\mu) \;=\; \frac{1}{2\pi i}\frac{H(\mu)}{2}\int_{-i\infty}^{i\infty} dp\; \bar{Q}(p)\frac{H(-1/p)}{1-\mu p}\;. \tag{53}$$

For the special case of an exponential source, we find

$$Q(x) \;=\; e^{-\alpha x}\;,\; \alpha \;>\; 0\;, \tag{54a}$$

which implies

$$\bar{Q}(p) \;=\; \frac{1}{p+\alpha}\;, \tag{54b}$$

Eq.(53) becomes upon evalution of the contour integral [$H(-1/p)$ has singularities in the right-half plane]

$$\phi(0,-\mu) \;=\; \frac{1}{2}\frac{H(\mu)H(1/\alpha)}{1+\alpha\mu}\;. \tag{55}$$

3.b. Scalar flux

From integral transport theory applied to eqs.(47), we find

$$\phi(0,-\mu) \;=\; \frac{c}{2\mu}\int_0^\infty dx'\; e^{-x'/\mu}\phi(x') \;+\; \frac{1}{2\mu}\int_0^\infty dx'\; e^{-x'/\mu}Q(x')\;. \tag{56}$$

Thus,

$$\phi(x) \;=\; \frac{2}{c}\mathcal{L}_x^{-1}\left[\phi(0,-1/s)/s\right] \;-\; \frac{Q(x)}{c} \tag{57}$$

with $\phi(0,-1/s)$ given by eq.(55); for the particular case of an exponential source

$$\phi(x) = \frac{1}{c}\left[H(1/\alpha)\mathcal{L}_x^{-1}\left\{\frac{H(1/s)}{s+\alpha}\right\} - e^{-\alpha x}\right] . \tag{58}$$

3.c. Angular flux

Taking a Laplace transform of eqs.(47) yields

$$\bar{\phi}(s,\mu) = \frac{c}{2}\frac{\bar{\phi}(s)}{1+\mu s} + \frac{1}{2}\frac{\bar{Q}(s)}{1+\mu s} + \frac{\mu}{1+\mu s}\phi(0,\mu) . \tag{59}$$

Since from eq.(57)

$$\bar{\phi}(s) = \frac{2}{c}\phi(0,-1/s)/s - \frac{\bar{Q}(s)}{c} ,$$

eq.(59) becomes

$$\bar{\phi}(s,\mu) = \frac{1}{1+\mu s}\left[\phi(0,-1/s)/s + \mu\phi(0,\mu)\right] ; \tag{60}$$

and, therefore, for $\mu > 0$

$$\bar{\phi}(s,\mu) = \phi(0,-1/s)/(s(1+\mu s)) \tag{61a}$$

$$\bar{\phi}(s,-\mu) = \frac{1}{1-\mu s}\left[\phi(0,-1/s)/s - \mu\phi(0,-\mu)\right] . \tag{61b}$$

For an exponential source again using eq.(55) for $\mu > 0$

$$\bar{\phi}(s,\mu) = \frac{1}{2}\frac{H(1/\alpha)H(1/s)}{(1+\mu s)(s+\alpha)} \tag{62a}$$

$$\bar{\phi}(s,-\mu) = \frac{1}{2}\frac{H(1/\alpha)}{1-\mu s}\left[\frac{H(1/s)}{s+\alpha} - \frac{H(\mu)}{\alpha+1/\mu}\right] \tag{62b}$$

with the angular flux recovered from eq.(46).

III. ADJACENT HALF-SPACE PROBLEMS

For some physical situations, especially in electron transport, interfacial effects between two media are important. For this reason, the adjacent half-space configuration will be investigated. The geometry consists of two adjacent half-spaces of differing scattering and absorbing properties. Several of the source configuratons of the previous section will be considered. Again the analytical solution are based on the solution to the beam albedo problem of § II.1.a.

III.1 Interfacial Flux Source

The spatial domain is extended to negative positions measured in units of the mean free paths of each medium. The transport equation to be solved in each medium (j=1,2) for an interfacial flux source is:

$$\left[\mu\frac{\partial}{\partial x} + 1\right]\phi_j(x,\mu) = \frac{c_j}{2}\int_{-1}^{1} d\mu'\phi_j(x,\mu') \tag{63a}$$

$$\phi_1(0,\mu) = \phi_2(0,\mu) + f(\mu) \tag{63b}$$

$$\lim_{x\to\infty}\phi_1(x,\mu) < \infty\ , \lim_{x\to-\infty}\phi_2(x,\mu) < \infty\ . \tag{63c}$$

The half-spaces are positioned as shown in Fig.1. Several flux source conditions $[f(\mu)]$ at $x=0$ will be considered in the following sections.

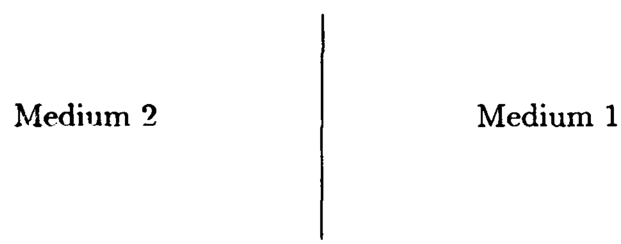

Figure 1

1.a Beam Interfacial Source

The analysis follows for a beam flux directed into medium 1:

$$f(\mu) = \delta(\mu - \mu_0) , \; \mu_0 > 0 . \tag{64}$$

i. Exiting flux

The analysis begins by reformulating eqs.(63) in terms of the collided and uncollided flux components. Thus, if

$$\phi_j(x, \mu; \mu_0) = \phi_{j,0}(x, \mu; \mu_0) + \phi_{j,c}(x, \mu; \mu_0) , \tag{65}$$

then

$$\phi_{j,0}(x, \mu; \mu_0) = \delta_{j,1} e^{-x/\mu_0} \delta(\mu - \mu_0) \tag{66}$$

and

$$\left[\mu \frac{\partial}{\partial x} + 1\right] \phi_{j,c}(x, \mu; \mu_0) = \frac{c_j}{2} \int_{-1}^{1} d\mu' \phi_{j,c}(x, \mu'; \mu_0) + \\ + \delta_{j,1} \frac{c_1}{2} e^{-x/\mu_0} \tag{67a}$$

$$\phi_{2,c}(0, \mu; \mu_0) = \phi_{1,c}(0, \mu; \mu_0) \tag{67b}$$

$$\lim_{x \to \infty} \phi_{1,c}(x, \mu; \mu_0) < \infty , \lim_{x \to -\infty} \phi_{2,c}(x, \mu; \mu_0) < \infty . \tag{67c}$$

The results of Prinja[7] are central to the analysis to follow. The solutions found in ref.7 are based on the solution to an integral equation formed

by considering each half-space separately with eq.(63b) serving as the connection. Eq.(30), with an appropriately defined $f(\mu)$ for each half-space, then provides a set of integral equation to be solved. The solution to these equations [letting $p = 1/\mu_0$ in eq.(48) of ref.7] for the exiting flux is

$$\phi_1(0,-\mu;\mu_0) = \frac{c_1 c_2}{2(c_2 - c_1)}\left[1 - \frac{c_1}{c_2}\frac{H_1(\mu_0)H_1(\mu)}{H_2(\mu_0)H_2(\mu)}\right]\frac{1}{1+\mu/\mu_0} \quad (68a)$$

$$\phi_2(0,\mu;\mu_0) = \frac{c_1 c_2}{2(c_2 - c_1)}\left[1 - \frac{H_1(\mu_0)H_2(\mu)}{H_2(\mu_0)H_1(\mu)}\right]\frac{1}{1-\mu/\mu_0}\;. \quad (68b)$$

In addition, a set of integral equations for $\phi_j(0,\mu;\mu_0)$ can be directly established by considering the incoming flux for each half-space to be known. For $\mu_0 > 0$ and using eq.(31) in medium 1 with

$$f(\mu) = \delta(\mu - \mu_0) + \phi_2(0,\mu;\mu_0) \quad (69)$$

and in medium 2 with

$$f(\mu) = \phi_1(0,-\mu;\mu_0) \quad (70)$$

gives

$$\phi_1(0,-\mu;\mu_0) = \frac{c_1}{2}\frac{\mu_0}{\mu+\mu_0}H_1(\mu_0)H_1(\mu) + $$

$$+ \frac{c_1}{2}H_1(\mu)\int_0^1 d\mu'\frac{\mu'}{\mu+\mu'}H_1(\mu')\phi_2(0,\mu';\mu_0) \quad (71a)$$

$$\phi_2(0,\mu;\mu_0) = \frac{c_2}{2}H_2(\mu)\int_0^1 d\mu'\frac{\mu'}{\mu+\mu'}H_2(\mu')\phi_1(0,-\mu';\mu_0)\;. \quad (71b)$$

This set of integral equations is numerically convenient as an alternative solution especially for $\mu = \mu_0$ and $c_1 = c_2$ when eqs.(68) become indeterminant and therefore difficult to evaluate. Also eqs.(71) can be used to generate the interfacial distributions for a general interfacial source $f(\mu)\theta(\mu)$ with ease:

$$\begin{aligned}\phi_1(0,-\mu) &= \frac{c_1}{2}H_1(\mu)\int_0^1 d\mu' \frac{\mu'}{\mu+\mu'} f(\mu')H_1(\mu') + \\ &+ \frac{c_1}{2}H_1(\mu)\int_0^1 d\mu' \frac{\mu'}{\mu+\mu'} H_1(\mu')\phi_2(0,\mu') \qquad (72a)\\ \phi_2(0,-\mu) &= \frac{c_2}{2}H_2(\mu)\int_0^1 d\mu' \frac{\mu'}{\mu+\mu'} H_2(\mu')\phi_1(0,-\mu') \;. \qquad (72b)\end{aligned}$$

ii. Scalar flux

When eqs.(63) for the beam flux source are reformulated using integral transport theory, there results at $x = 0$

$$\phi_1(0,-\mu;\mu_0) = \frac{c_1}{2\mu}\int_0^\infty dx'\; e^{-x'/\mu}\phi_1(x';\mu_0) \qquad (73a)$$

$$\phi_2(0,\mu;\mu_0) = \frac{c_2}{2\mu}\int_0^\infty dx'\; e^{-x'/\mu}\phi_2(-x';\mu_0) \qquad (73b)$$

which implies

$$\phi_1(x;\mu_0) = \frac{2}{c_1}\mathcal{L}_x^{-1}\left[\phi_1(0,-1/s;\mu_0)/s\right] \qquad (74a)$$

$$\phi_2(-x;\mu_0) = \frac{2}{c_2}\mathcal{L}_x^{-1}\left[\phi_2(0,1/s;\mu_0)/s\right] \qquad (74b)$$

where $\phi_j(0,\mp 1/s;\mu_0)$ are given by eqs.(68) or (71).

iii. Angular flux

From the Laplace transform of eqs.(63) for $0 \leq x$ when $j = 1$ and $x \leq 0$ when $j = 2$ respectively, we have

$$\bar{\phi}_j(s, \mu; \mu_0) \;=\; \frac{1}{1+\mu s}\left[\frac{c_j}{2}\bar{\phi}_j(s; \mu_0) \;+\; \mu\phi_j(0, \mu; \mu_0)\right] \tag{75}$$

where

$$\bar{\phi}_1(s, \mu; \mu_0) \;\equiv\; \int_0^\infty dx\; e^{-sx}\phi_1(x, \mu; \mu_0)$$

$$\bar{\phi}_2(s, \mu; \mu_0) \;\equiv\; \int_0^\infty dx\; e^{-sx}\phi_2(-x, \mu; \mu_0)$$

with

$$\bar{\phi}_j(s; \mu_0) \;=\; \frac{2}{c_j}\phi_j(0, \mp 1/s; \mu_0)/s \tag{76}$$

where $\mp(-,+)$ is for $j = 1, 2$ respectively, and eq.(75) becomes

$$\bar{\phi}_j(s, \mu; \mu_0) \;=\; \frac{1}{1+\mu s}\left[\phi_j(0, \mp 1/s; \mu_0)/s \;+\; \mu\phi_j(0, \mu; \mu_0)\right] \,. \tag{77}$$

The inversion is then given by eq.(46) to provide the angular flux in each half-space.

III.2 Milne Problem

Because the adjacent half-space Milne problem is well documented in the literature[8], only the results will be presented in this section.

i. Interfacial flux

For this case the source is assumed to be at infinity in medium 1 yielding

$$\phi_1(0,-\mu) = \frac{c_1}{2}\frac{\nu_{0,1}}{\nu_{0,1}-\mu}\frac{H_1(\mu)}{H_2(\mu)}\frac{H_2(\nu_{0,1})}{H_1(\nu_{0,1})} \tag{78a}$$

$$\phi_2(0,\mu) = \frac{c_2}{2}\frac{\nu_{0,1}}{\nu_{0,1}+\mu}\frac{H_2(\mu)}{H_1(\mu)}\frac{H_2(\nu_{0,1})}{H_1(\nu_{0,1})} \tag{78b}$$

where $\nu_{0,1}$ satisfies eq.(35c) with c replaced by c_1.

ii. Scalar flux

Again form integral transport theory, one finds

$$\phi_1(x) = \frac{2}{c_1}\mathcal{L}_x^{-1}\left[\phi_1(0,-1/s)/s\right] \tag{79a}$$

$$\phi_2(-x) = \frac{2}{c_2}\mathcal{L}_x^{-1}\left[\phi_2(0,1/s)/s\right] \; . \tag{79b}$$

with $\phi_j(0,\mp 1/s)$ given by eqs.(78).

iii. Angular flux

As in the previous case, eqs.(77) apply for $\mu > 0$

$$\bar{\phi}_j(s,\mu) = \frac{1}{1+\mu s}\left[\phi_j(0,\mp 1/s)/s \; + \; \mu\phi_j(0,\mu)\right] \; , \tag{80}$$

and the angular flux is obtained by Laplace transform inversion.

II.3 Spatially Distributed Source

Here, we assume a spatially distributed isotropic source exists in the right half-space ($j = 1$) only. Thus, the transport equation to be solved is

$$\left[\mu\frac{\partial}{\partial x} + 1\right]\phi_j(x,\mu) = \frac{c_1}{2}\int_{-1}^{1} d\mu'\phi_j(x,\mu') + \delta_{j,1}\frac{Q(x)}{2} \qquad (81a)$$

$$\phi_1(0,\mu) = \phi_2(0,\mu) \qquad (81b)$$

$$\lim_{x\to\infty}\phi_1(x,\mu) < \infty \, , \lim_{x\to-\infty}\phi_2(x,\mu) < \infty \, . \qquad (81c)$$

For $\mu_0 > 0$, the transport equations for a beam flux source for the collided contribution are given by eqs.(67). As for the single half-space case, if μ_0 is replaced by $-1/p$ and eqs.(67) are operated upon by eq.(50) where $\bar{Q}(p)$ has singularities only in the left-half of the complex p-plane, then it can be shown that for $j = 1, 2$

$$\phi_j(x,\mu) = \frac{1}{2\pi i}\frac{1}{c_1}\int_{-i\infty}^{i\infty} dp\ \bar{Q}(p)\phi_{j,c}(x,\mu,-1/p) \qquad (82)$$

satisfies eqs.(81). The exiting scalar and angular flux for this case will be obtained for an exponential source only [see eqs.(54)].

i. Exiting flux

Since

$$\bar{Q}(p) = \frac{1}{p+\alpha} \, , \qquad (83)$$

the contour integration in eqs.(82) yields for $\mu > 0$

$$\phi_1(0,-\mu) = \phi_{1,c}(0,-\mu;1/\alpha)/c_1 \tag{84a}$$

$$\phi_2(0,\mu) = \phi_{2,c}(0,\mu;1/\alpha)/c_1 \tag{84b}$$

where $\phi_{j,c}(0,\mu,1/\alpha)$ for $j=1,2$ are given by eqs.(68) or (71) with μ_0 replaced by $1/\alpha$.

ii. Scalar flux

As in § III.1.a.ii and II.3.b

$$\phi_1(x) = \frac{1}{c_1}\left\{\frac{2}{c_1}\mathcal{L}_x^{-1}\left[\phi_{1,c}(0,-1/s;1/\alpha)/s\right] - e^{-\alpha x}\right\} \tag{85a}$$

$$\phi_2(-x) = \frac{2}{c_1 c_2}\mathcal{L}_x^{-1}\left[\phi_{2,c}(0,1/s;1/\alpha)/s\right] \ . \tag{85b}$$

iii. Angular flux

The transform of the angular flux is given by

$$\bar{\phi}_j(s,\mu) = \frac{1}{1+\mu s}\left[\phi_{j,c}(0,\mp 1/s;1/\alpha)/s \ + \ \mu\phi_{j,c}(0,\mu;1/\alpha)\right] \ ; \tag{86}$$

and finally the inversion is obtained from eq.(46) in each half-space.

IV. Numerical Implementation and Demonstration

At the heart of the numerical evaluation of the exiting, scalar and angular flux lies the evaluation of the $H-$function. Currently, there exists several methods for evaluating the $H-$function including the evaluation of

- the analytical representation as provided by the Wiener-Hopf solution to eq.(15)
- the multiple collision solution to eq.(15)
- approximate represention s
- eq.(15) directly by iteration.

It is the last method which has proven to be the most reliable as well as most efficient.

The method begins with the discretization of the μ variable using the Gauss-quadrature[9]. By approximating the integral in eq.(15) with a shifted Legendre-Gauss quadrature of order L_m and evaluating the resultant equation at the quadrature abcissae, the following iteration scheme results:

$$H_j^{k+\frac{1}{2}} = \left[1 - \frac{c}{2}\mu_j \sum_{m=1}^{L_m} \omega_{m} \frac{H_m^k}{\mu_m + \mu_j}\right]^{-1} \tag{87}$$

where

$$H_m^k \equiv H^k(\mu_m) \ , \ H_m^{k+\frac{1}{2}} \equiv H^{k+\frac{1}{2}}(\mu_m) \ . \tag{88}$$

The full iteration step is accomplished via satisfying the zeroth moment:

$$H_j^{k+1} = \left[\frac{\alpha_0}{\tilde{\alpha}_0}\right] H_j^{k+\frac{1}{2}} \tag{89}$$

with

$$\tilde{\alpha}_0 \equiv \sum_{m=1}^{L_m} \omega_m H_m^{k+\frac{1}{2}} . \qquad (90)$$

The second numerical procedure of importance is the numerical Laplace transform inversion. The numerical inversion is obtained through the following steps:

- transformation of the Bromwich contour formulation

$$f(t) = \frac{1}{2\pi i} \int_{\gamma - i\infty}^{\gamma + i\infty} ds\; e^{st} \bar{f}(s) , \qquad (91)$$

where γ is greater than the largest real part of any singularity of the image function $f(s)$, into the cosine integral

$$f(t) = \frac{2e^{\gamma t}}{\pi t} \int_0^{\infty} dw\; \Re\left\{\bar{f}(\gamma + iw/t)\right\} \cos(w) \qquad (92)$$

- reformulation of the infinite integral into an infinite series

$$f(t) = \sum_{k=0}^{\infty} (-1)^k \int_0^{\pi} dw\; \Re\{\bar{f}(\gamma + (w + ik\pi)/t)\} \cos(w) \qquad (93)$$

- evaluation of the integral in eq.(93) with the Romberg integration rule[10]

- acceleration of the convergence of the infinite series through either the epsilon or the Euler-Knopp[9] acceleration algorithm.

Finally, in some cases, it is desirable to solve the integral equations given by eqs.(71) rather than use the analytical expressions of eqs.(68). This is simply done by discretization and subsequent matrix inversion.

Figures 2-6 are presented as a demonstration of the evaluation of the scalar flux for a selected set of problems. While only curves are presented

here, the scalar fluxes for all cases considered in this report can be obtained to 5-place accuracy or better. Thus, the numerical Laplace transform inversion represents a true analytical benchmark.

Figure 2 gives the flux for the albedo problem for a normally incident beam flux. The number of secondaries c has been specified to be $c = 0.1(0.2)0.9$. Note the exponential decrease far form the surface, as one would expect, and the change of the sign of the derivative with c at $x = 0$. Figure 3 provides the flux for the same variation of c for the Milne problem. This time the flux increases exponentially at large distances and deviates from exponential behavior near the medium surface. Figure 4 shows the behavior of the scalar flux for a spatially distributed exponential source given by eq.(54a) with $\alpha = 0.0(0.5)2.0$. For $\alpha = 0$, the source is uniform and the flux can be shown to asymptotically approach $1/(1-c)$ which, in this case, is 10.

Finally, Figs.5 and 6 give the scalar flux in two adjacent half-spaces. Figure 5 depicts the flux for the Milne problem for a variation of $c_2 = 0.1(0.2)0.9$ in medium 2 and $c_1 = 0.9$ in medium 1. Note the strong purturbation of the flux near the interface. Figure 6 gives the scalar flux for a uniformly distributed source ($\alpha = 0$ in medium 1) for a variation of $c_2 = 0.1(0.2)0.9$. Again the scalar flux approaches $1/(1-c_1)$ asymptotically.

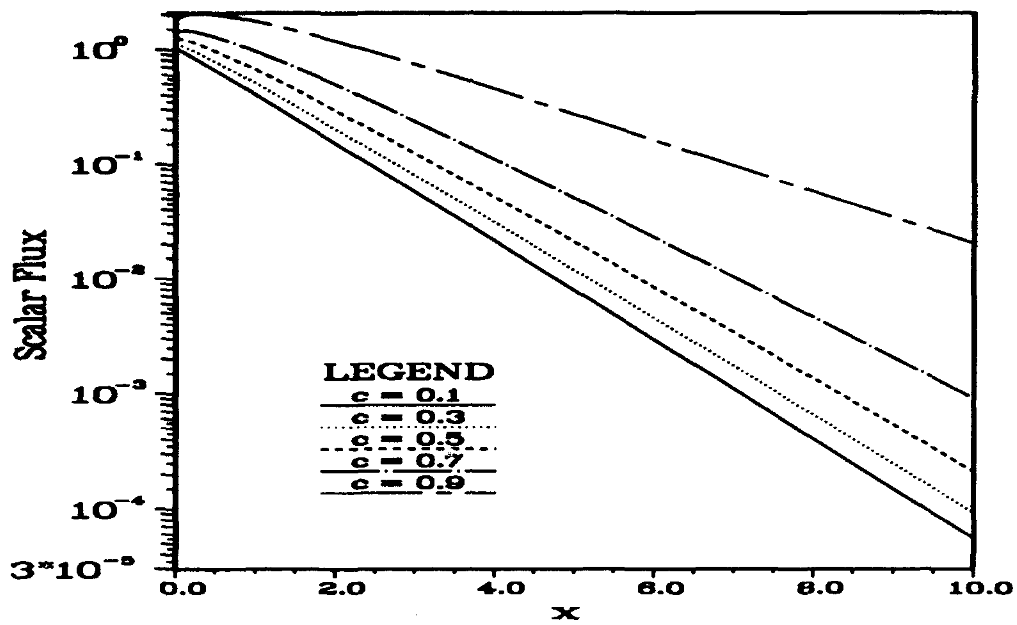

Fig.2 Variation of c for albedo problem with beam source $\mu_0 = 1$

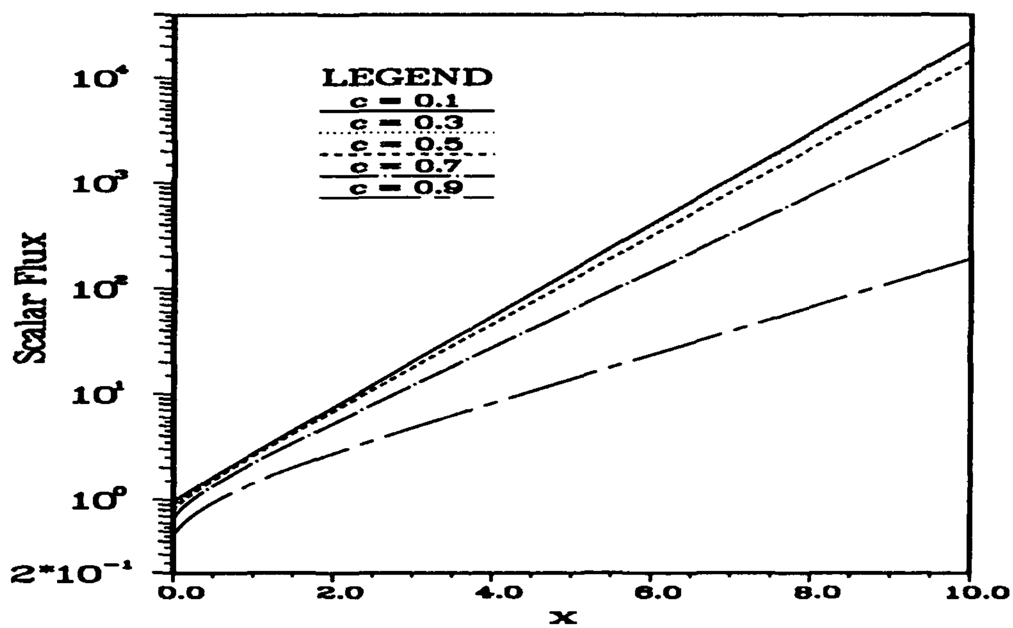

Fig.3 Variation of c for Milne problem

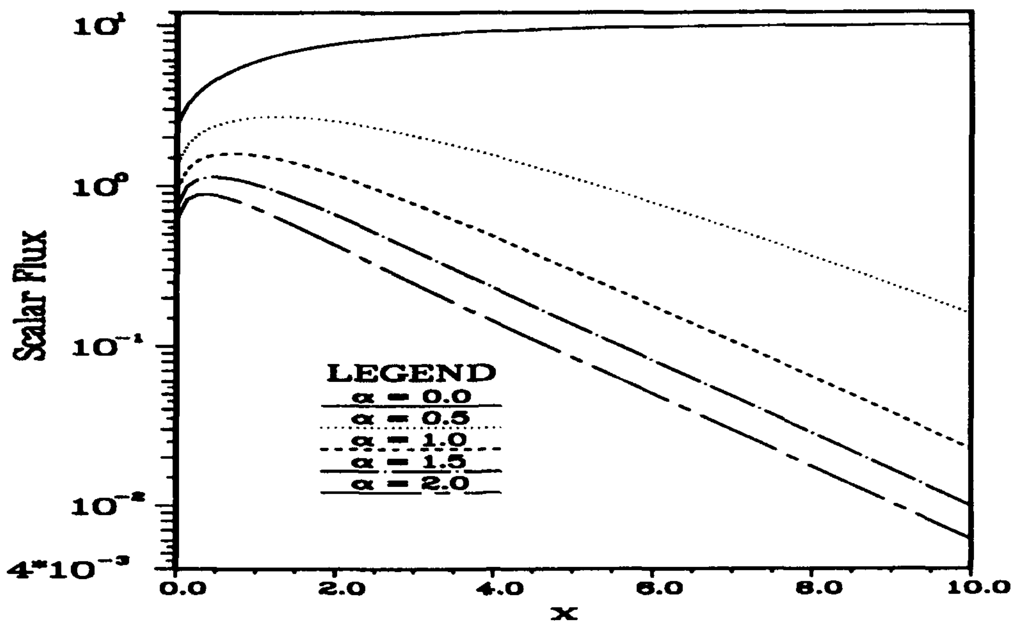

Fig.4 Variation of α for distributed source $e^{-\alpha x}$, $c = 0.9$

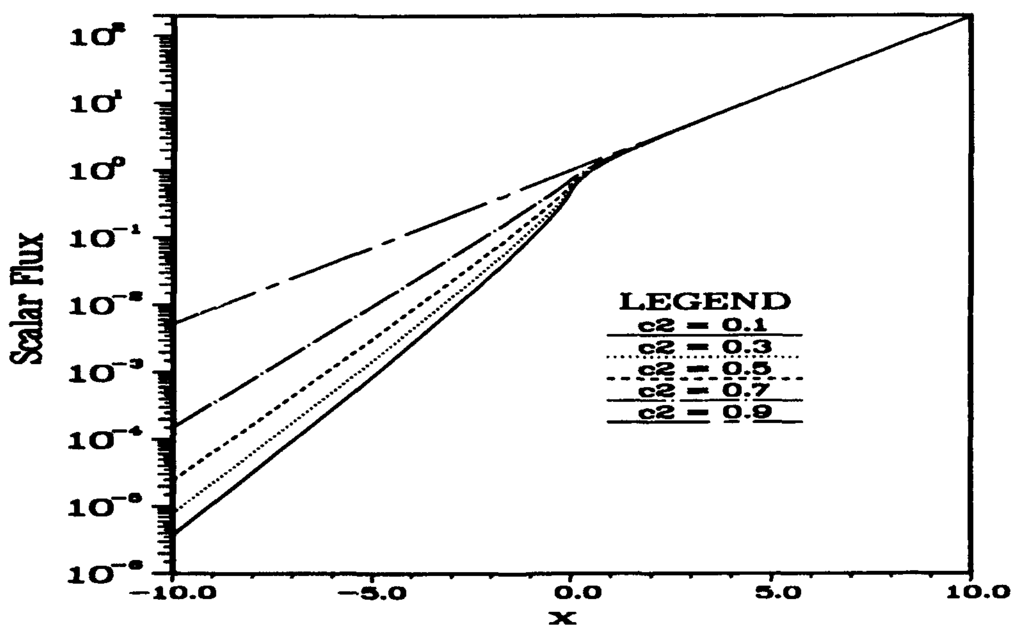

Fig.5 Variation of c_2 for adjacent half-space Milne problem, $c_1 = 0.9$

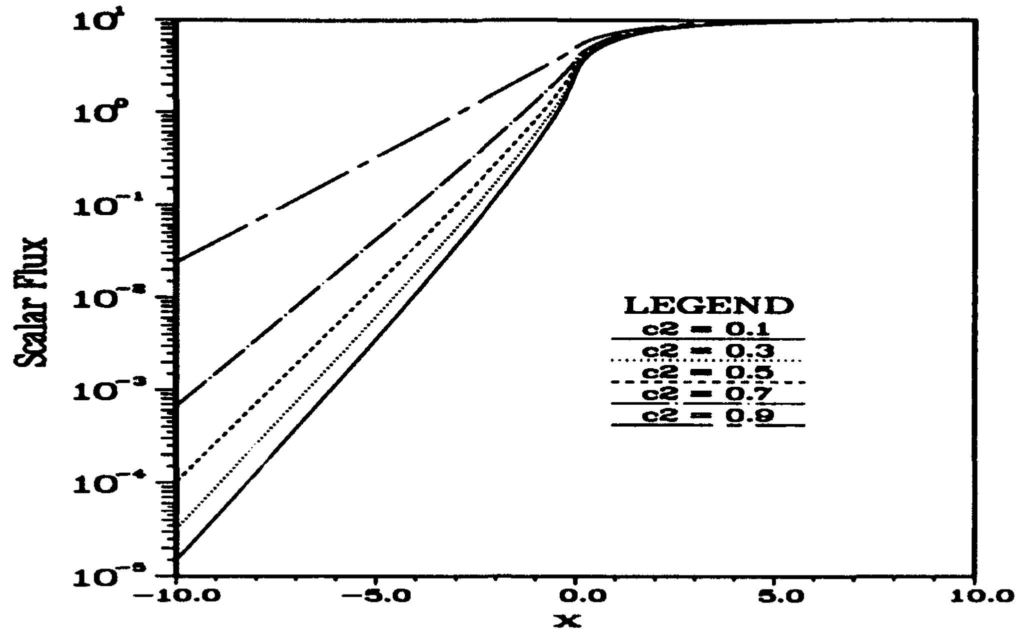

Fig.6 Variation of c_2 for adjacent half-space uniform source in medium 1 problem, $c_1 = 0.9$

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APPENDIX A

Some Useful Relations for the H-Function

There exists several useful relations satisfied by the $H-$function which are required to perform $H-$function calculus. These include:

A.1 Zeroth moment

$$\alpha_0 = \int_0^1 d\mu' H(\mu') = \frac{2}{c}\left[1 - \sqrt{1-c}\,\right] \tag{A.1}$$

A.2 An integral relation

$$I_1 \equiv \frac{c}{2}H(\mu)\int_0^1 d\mu' \frac{\mu'}{\mu+\mu'}H(\mu') = 1 - \sqrt{1-c}\,H(\mu) \tag{A.2}$$

APPENDIX B

Description of SEMI1 Program for the Determination of Fluxes in a Semi-infinite Medium

B.1 General Description

The SEMI1 program (version 1) has been developed to treat neutral particle transport in a semiinfinite medium. The analytical solution to the transport equation for single and two half space geometries for a variety of sources is evaluated numerically. The angular flux at $x = 0$ is evaluated using expressions derived from Chandrasekhar's Principles of Invariance. The scalar flux in the interior is evaluated using these expressions as image functions for a Laplace transform inversion performed numerically as discussed above. Six source configurations are considered for each half-space geometry.

B.2 Specific Description

B.2.1 Input

The input to the program is as follows:

input description(free format)

line 1			
	nc	number of cases	
line 2			
	lj	number of terms in inversion series (<100)	
	lg	number of iterations of bromwich contour (<10)	
	gt	to determine starting contour gam0 (0.1)	
line 3			
	x0	initial edit position from x=0	
	xl	final edit position from x=0	
	nx	number of intervals between x0 and xl (<m2)	
	iflux	0 exiting angular flux only	
		1 interior scalar flux only	
		2 both exiting angular and scalar fluxes	
	anl	limiting direction for angular edit (-anl,anl)	
	mx	number of edit points (<m1)	
note: repeat line 4 for the nc cases			
	single half-space geometry:		
line 4	is	1	beam source
		2	isotropic source
		3	Milne problem
		4	uniformly distributed isotropic source
		5	distributed isotropiexponential source
		6	general angular distribution at surface
	two half-spaces geometry:		
		51	beam flux at interface
		52	half range source at interface
		53	Milne problem
		54	uniformly distributed source in right half-space
		55	distributed isotropic exponential source in right half-space
		56	general angular distribution at interface
	q0	source normalization	
	al	exponent of exponential source	
	be	exponent for general angular source (ff=e**(-be/(1-mu**2)))	
	c1	number of secondaries in right-space	
	c2	number of secondaries in left-space	
	am0	source direction	
	lm	Gauss-Legendre quadrature order(<m1)	
	err	desired relative error	

a) Notes:

1) The number of cases **nc** considered is unlimited.

2) The number of spatial and angular edit points **nx,mx** is currently limited to 100 for the single half-space and 200 for two half-spaces but can be changed by specifying m1 and m2 in the program.

3) **lj** is the maximum number of terms allowed in the inversion series; while **lg** specifies the maximum number of contours on which the inversion is evaluated in order to achieve convergence.

4) **gt** specifies the Bromwich contour $\gamma = \gamma_s + \mathbf{gt}/x$ when x is less than 0.1 and is the initial contour otherwise. γ_s is an approximation to the real part of the rightmost singularity.

5) The general angularly dependent source currently used is

$$f(\mu) = Q_0 e^{-\beta/(1-\mu^2)}$$

where β is input as **be** and Q_0 is determined from normalization.

6) The maximum Gauss-Legendre quadrature order is m1

B.2.2 Output

The exiting or interfacial angular flux and the interior scalar flux are output on files *eang* and *scal* respectively. Diagnostic messages found on file *o3* are as follows:

tape23 (o3) diagnostic messages:

a) error 0: h-function iteration did not converge
b) error 1a,b: search for zero of infinite medium dispersion relation did not converge
c) error 2: x=aaaaa err=bbbbb: inversion series did not converge at x=aaaaa with error estimate err=bbbbb
d) error 3: possible loss of accuracy in inversion series
e) error 4: j=iiiii x=aaaaa err=bbbbb: Romberg integration did not converge at term j and x=aaaaa with error estimate err=bbbbb
f) error 5: x=aaaaa err=bbbbb: contour iteration did not converge at x=aaaaa with error estimate err=bbbbb
g) error 6: search for zeros of the Legendre polynomial failed

while files *o4* and *o5* are plot files for the interior scalar flux and angular flux at $x = 0$ respectively. The number of contours for convergence is monitored on the screen. The completion of each case is signaled by an indication of the files which have been written.

B.2.3 Program Notes

1) Loss of accuracy

   Since the inversion is performed by summing a series, there is always the possibility of loss of accuracy. To partially offset this difficulty, an iterative procedure has been introduced. If such a loss is sensed by the sum being less than any one term, the error in the Romberg integration is reduced to obtain more accuracy for the terms of the series. The computation is then repeated.

2) Nonconvergence

   If the inversion does not converge for small x ($x < 0.1$), **gt** should be increased in an attempt to achieve convergence. In general, the inversion cannot give values smaller then machine accuracy. Sometimes by judicious a choice of the contour, smaller values can be obtained however.

MISSION

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